

# Mode coupling theory for sheared granular liquids

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**Abstract.** Sheared granular liquids are studied by the mode coupling theory. It is shown that, in contrast to thermostatted systems, current correlations play an essential role in the dynamics. The theory predicts that the plateau of the density time-correlator disappears for most situations, while it appears in the elastic limit. The result is compatible with molecular dynamics simulations.

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## INTRODUCTION

It is believed in the description of granular flows that the kinetic theory of Boltzmann-Enskog is applicable up to volume fraction  $\phi \leq 0.5$  [1, 2, 3, 4, 5]. However, any reliable theory for dense granular flows with  $\phi > 0.5$  does not exist, where the picture of instantaneous collision breaks down. Experiments and simulations suggest that the constitutive equation of the shear stress exhibits a crossover from the Bagnold law to a power-law behavior with a non-trivial exponent, and eventually results in a yield stress for large  $\phi$  [6, 7]. To understand this behavior by a first-principle theory is desired.

On the other hand, Liu and Nagel [8] suggested the existence of a closed relationship between the jamming transition and the glass transition. Since then, to clarify this relation has been one of the hottest subjects in both granular and glassy physics [9]. This situation has motivated us to apply the mode coupling theory (MCT) [10] successfully used for glassy materials to granular materials [11, 12]. This is in accordance with the establishment of the notion of “granular liquids” [13, 14, 15, 16], where long-time, long-range correlations are significant, as well as in molecular liquids. Hayakawa and Otsuki [11] introduced a MCT for sheared granular liquids of hard-core inelastic spheres, but realistic granular grains are soft and the application of the pseudo-Liouillian [1] is unnecessary. Kranz *et al.* [12] studied MCT for driven inelastic spheres with a Gaussian white-noise thermostat, but the correspondence of their model with the actual vibrating granular systems, which incorporate non-Gaussian mechanical forces, is quite unclear.

With the above situation in consideration, we attempt to construct a liquid theory for sheared granular spheres with a soft-core potential, starting from the Liouville equation [17, 18, 19, 20]. In particular, we apply the MCT to obtain a set of closed equations for the time-

correlators. Although MCT is still not completely established as a theory of glasses, its problem is not serious at least for sheared systems, so we adopt the conventional approach of projection operators and the Mori-type equations [21, 22]. The physical significance of the current correlation is demonstrated by exhibiting its effect on the slow dynamics.

## FORMULATION

In this section, we present the equation of motions for the time-correlators (MCT equation). Detailed derivations for the basic formulation of sheared underdamped MCT can be found in Ref. [23], so we focus on the issues specific to granular systems.

Our microscopic starting point is the SLLOD equation [24] for a system under a uniform and stationary shear with  $N$  spherical particles of mass  $m$  and diameter  $d$ ,

$$\dot{\mathbf{r}}_i(t) = \frac{\mathbf{p}_i(t)}{m} + \boldsymbol{\kappa} \cdot \mathbf{r}_i(t), \quad (1)$$

$$\dot{\mathbf{p}}_i(t) = \mathbf{F}_i^{(\text{el})}(t) + \mathbf{F}_i^{(\text{dis})}(t) - \boldsymbol{\kappa} \cdot \mathbf{p}_i(t), \quad (2)$$

where  $\kappa^{\lambda\mu} = \dot{\gamma} \delta^{\lambda x} \delta^{\mu y}$  is the  $\lambda\mu$  component of the shear-rate tensor ( $\lambda, \mu = x, y, z$ ),  $\dot{\gamma}$  is the shear rate,  $\mathbf{F}_i^{(\text{el})}$  is the conservative force with a soft-core potential,  $\mathbf{F}_i^{(\text{dis})} = \sum_{j \neq i} \mathbf{F}_{ij}^{(\text{dis})}$  is the viscous dissipative force, where  $\mathbf{F}_{ij}^{(\text{dis})}$  is the pairwise contact dissipative force,

$$\mathbf{F}_{ij}^{(\text{dis})} = -\hat{\mathbf{r}}_{ij} \mathcal{F}(r_{ij}) (\mathbf{v}_{ij} \cdot \hat{\mathbf{r}}_{ij}), \quad (3)$$

$$\mathcal{F}(r_{ij}) \equiv \zeta \Theta(d - r_{ij}), \quad (4)$$

with  $\mathbf{v}_{ij} \equiv \mathbf{v}_i - \mathbf{v}_j$ ,  $\mathbf{r}_{ij} \equiv \mathbf{r}_i - \mathbf{r}_j$ ,  $r_{ij} \equiv |\mathbf{r}_{ij}|$ ,  $\hat{\mathbf{r}}_{ij} \equiv \mathbf{r}_{ij}/r_{ij}$ , and  $\Theta(x)$  is the Heaviside's step function, where  $\Theta(x) = 1$  for  $x > 0$  and  $\Theta(x) = 0$  otherwise. Here,  $\zeta$  is the bare

viscous coefficient which is directly related to the restitution coefficient. We consider frictionless granular materials to avoid the complexity to treat the Coulomb friction and the rotation of grains. The uniform shear velocity (in the  $x$ -direction) is  $v_{\text{sh}}(y) = \dot{\gamma}y$ , and the distance of the two shear boundaries is denoted as  $L$ . Hence, the velocity at the boundaries may satisfy  $v_0^{(\pm)} \equiv \pm L\dot{\gamma}/2$ . The system is assumed to be in equilibrium before time  $t = 0$ , and shearing and interparticle dissipation are turned on at  $t = 0$ , after which a steady-state is asymptotically reached for  $t \rightarrow \infty$ .

It is possible to recast the SLLOD equation, Eqs. (1) and (2), into the Liouville equation, and successively by the application of the projection operator [20],  $\mathcal{P}(t) = \sum_{\mathbf{k}} \langle X n_{\mathbf{k}(t)}^* \rangle / (N S_{k(t)} n_{\mathbf{k}(t)} + \sum_{\mathbf{k}} \langle X j_{\mathbf{k}(t)}^{\lambda*} \rangle / (N v_T^2) j_{\mathbf{k}(t)}^{\lambda})$ , to derive the Mori-type equation for the time-correlators. Here,  $n_{\mathbf{q}} \equiv \sum_{i=1}^N e^{i\mathbf{q} \cdot \mathbf{r}_i} - N \delta_{\mathbf{q},0}$  and  $j_{\mathbf{q}}^{\lambda} \equiv \sum_{i=1}^N p_i^{\lambda} e^{i\mathbf{q} \cdot \mathbf{r}_i} / m$  are the density and current-density fluctuations, respectively, with  $\mathbf{q}(t) \equiv (q_x, q_y - \dot{\gamma}t q_x, q_z)$ , and  $v_T \equiv \sqrt{T/m}$  is the thermal velocity at the initial equilibrium state. In granular liquids, it is essential to include the projection onto the density-current modes  $\mathcal{P}_{nj}(t)$ , where

$$\mathcal{P}_{nj}(t)X \equiv \sum_{\mathbf{k} > \mathbf{p}} \frac{\langle X n_{\mathbf{k}(t)}^* j_{\mathbf{p}(t)}^{\lambda*} \rangle}{N^2 S_{k(t)} v_T^2} n_{\mathbf{k}(t)} j_{\mathbf{p}(t)}^{\lambda}, \quad (5)$$

to the second projection operator  $\mathcal{P}_2(t)$  as [25]

$$\mathcal{P}_2(t) = \mathcal{P}_{nn}(t) + \mathcal{P}_{nj}(t) \quad (6)$$

to obtain a closure for the Mori-type equation, where  $\mathcal{P}_{nn}(t)X \equiv \sum_{\mathbf{k} > \mathbf{p}} \langle X n_{\mathbf{k}(t)}^* n_{\mathbf{p}(t)}^* \rangle / (N^2 S_{k(t)} S_{p(t)}) n_{\mathbf{k}(t)} n_{\mathbf{p}(t)}$  is the conventional projection onto the pair-density modes. This choice of  $\mathcal{P}_2(t)$  requires us to consider, in addition to the conventional time-correlators  $\Phi_{\mathbf{q}}(t) \equiv \langle n_{\mathbf{q}(t)}(t) n_{\mathbf{q}}^* \rangle / N$  and  $H_{\mathbf{q}}^{\lambda}(t) \equiv i \langle j_{\mathbf{q}(t)}^{\lambda}(t) n_{\mathbf{q}}^* \rangle / N$ , two additional time-correlators,

$$\bar{H}_{\mathbf{q}}^{\lambda}(t) \equiv \frac{i}{N} \langle n_{\mathbf{q}(t)}(t) j_{\mathbf{q}}^{\lambda*} \rangle, \quad (7)$$

$$C_{\mathbf{q}}^{\lambda\mu}(t) \equiv \frac{1}{N} \langle j_{\mathbf{q}(t)}^{\lambda}(t) j_{\mathbf{q}}^{\mu*} \rangle. \quad (8)$$

These time-correlators turn out to play essential and significant roles in granular liquids.

## Isotropic approximation

It is almost hopeless to deal with four time-correlators with tensor indices. Hence, we attempt to reduce the degrees of freedom by applying the isotropic approximation. Since dissipation occurs irrespective of the

anisotropy of the strain, application of this approximation is expected not to be fatal.

Based on the isotropic approximation, it is able to reduce the vector/tensor time-correlators into two scalar time-correlators,  $\{\Phi_{\mathbf{q}}(t), \Psi_{\mathbf{q}}(t)\}$ . In particular,  $H_{\mathbf{q}}^{\lambda}(t)$  is reduced to  $H_{\mathbf{q}}^{\lambda}(t) \simeq q^{\lambda}(t) \frac{d}{dt} \Phi_{\mathbf{q}}(t) / q(t)^2$  as usual [23], and  $\bar{H}_{\mathbf{q}}^{\lambda}(t)$  to [26]

$$\bar{H}_{\mathbf{q}}^{\lambda}(t) \simeq -q^{\lambda}(t) \Psi_{\mathbf{q}}(t). \quad (9)$$

The correlator  $C_{\mathbf{q}}^{\lambda\mu}(t)$  is reduced to  $C_{\mathbf{q}}^{\lambda\mu}(t) \simeq C_q(t) \delta^{\lambda\mu}$  [26], where  $C_q(t)$  is written in terms of  $\Psi_q(t)$  as

$$C_q(t) = \frac{d}{dt} \Psi_q(t) + \frac{1}{2} \frac{\Psi_q(t)}{q(t)^2} \frac{d}{dt} q(t)^2. \quad (10)$$

The resulting MCT equations in the weak-shear regime read

$$\begin{aligned} \frac{d^2}{dt^2} \Phi_q(t) &= -v_T^2 \frac{q(t)^2}{S_{q(t)}} \Phi_q(t) - A_{q(t)} \frac{d}{dt} \Phi_q(t) \\ &\quad - \int_0^t ds \bar{M}_{q(s)}(t-s) \frac{d}{ds} \Phi_q(s), \end{aligned} \quad (11)$$

$$\begin{aligned} \frac{d^2}{dt^2} \Psi_q(t) &= -\frac{v_T^2}{3} \frac{q(t)^2}{S_{q(t)}} \Psi_q(t) - \frac{1}{3} A_{q(t)}^{\lambda\lambda} \frac{d}{dt} \Psi_q(t) \\ &\quad - \frac{1}{3} \int_0^t ds \bar{M}_{q(s)}^{\lambda\lambda}(t-s) \frac{d}{ds} \Psi_q(s), \end{aligned} \quad (12)$$

where

$$A_{\mathbf{q}} = \frac{4\pi}{3} \frac{n}{m} \int_0^{\infty} dr r^2 g(r) \mathcal{F}(r) [1 - j_0(qr) + 2j_2(qr)], \quad (13)$$

with the spherical Bessel function  $j_n(x)$  ( $n = 0, 2$ ), and

$$A_{\mathbf{q}}^{\lambda\lambda} = 4\pi \frac{n}{m} \int_0^{\infty} dr r^2 g(r) \mathcal{F}(r) [1 - j_0(qr)] \quad (14)$$

are the effective viscous coefficients. Here,  $n$  is the average density. In the weak-shear regime, we keep terms up to linear order in the shear rate  $\dot{\gamma}$  and the bare viscous coefficient  $\zeta$ , and neglect quadratic and higher terms. For instance,  $C_q(t)$  is approximated as  $C_q(t) \simeq d\Psi_q(t)/dt$ . Note that  $\mathcal{F}(r)$  incorporates  $\zeta$ , cf. Eq. (4). According to the choice of  $\mathcal{P}_2(t)$  in Eq. (6), there appear four terms in the memory kernels  $\bar{M}_{\mathbf{q}}(\tau)$  and  $\bar{M}_{\mathbf{q}}^{\lambda\lambda}(\tau)$ , respectively. A complete description of these terms is rather lengthy, so we report it elsewhere [25], and only show the explicit forms of  $\bar{M}_{\mathbf{q}}(\tau)$  for illustration. Among the four terms in  $\bar{M}_{\mathbf{q}}(\tau)$ ,

$$\bar{M}_{\mathbf{q}}(\tau) = \sum_{i=1}^4 \bar{M}_{\mathbf{q}}^{(i)}(\tau), \quad (15)$$

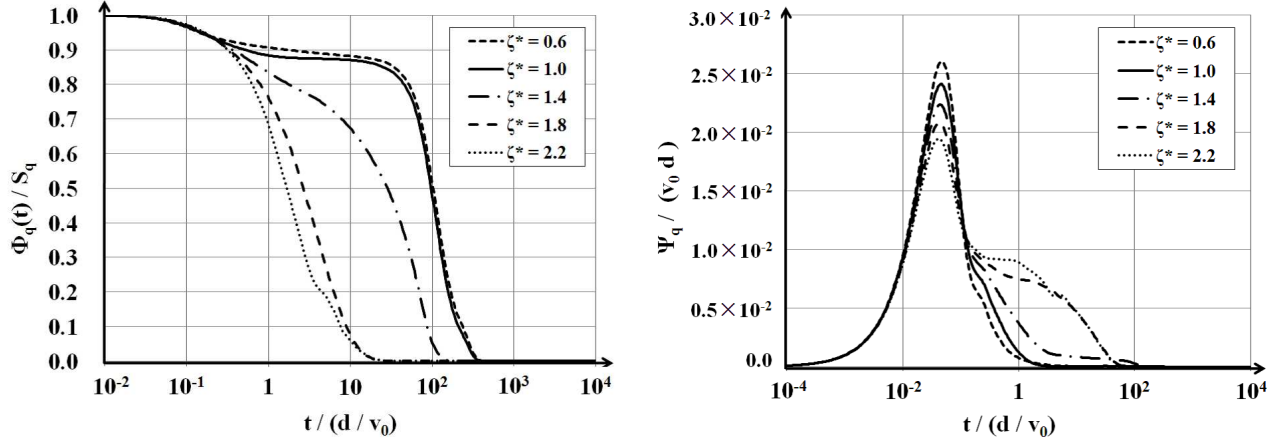


FIGURE 1. Numerical results for the density time-correlator (left) and the density-current time-correlator (right).

the first term  $\bar{M}_q^{(1)}(\tau)$  is the conventional term quadratic in  $\Phi_q(t)$ ,

$$\bar{M}_q^{(1)}(\tau) = \frac{nv_T^2}{2q^2} \int \frac{d^3\mathbf{k}}{(2\pi)^3} V_{q(\tau),\mathbf{k}(\tau),\mathbf{p}(\tau)}^{(\text{el})} V_{q,\mathbf{k},\mathbf{p}}^{(\text{el})} \Phi_k(\tau) \Phi_p(\tau), \quad (16)$$

which is responsible for the plateau of the density time-correlator. The other three terms originate in dissipation, where the two of them are given by

$$\begin{aligned} \bar{M}_q^{(2)}(\tau) &\simeq \frac{1}{q^2} \int \frac{d^3\mathbf{k}}{(2\pi)^3} \frac{p^\lambda(\tau)}{p(\tau)^2} V_{q(\tau),\mathbf{k}(\tau),\mathbf{p}(\tau)}^{(\text{vis})\lambda} V_{q,\mathbf{k},\mathbf{p}}^{(\text{el})} \\ &\quad \times \Phi_k(\tau) \frac{d}{d\tau} \Phi_p(\tau), \end{aligned} \quad (17)$$

$$\begin{aligned} \bar{M}_q^{(3)}(\tau) &\simeq -\frac{1}{q^2} \int \frac{d^3\mathbf{k}}{(2\pi)^3} V_{q(\tau),\mathbf{k}(\tau),\mathbf{p}(\tau)}^{(\text{el})} p^\lambda V_{q,\mathbf{k},\mathbf{p}}^{(\text{vis})\lambda} \\ &\quad \times \Phi_k(\tau) \Psi_p(\tau), \end{aligned} \quad (18)$$

and the remaining  $\bar{M}_q^{(4)}(\tau)$  is neglected since it is quadratic in  $\zeta$ . Here,  $V_{q,\mathbf{k},\mathbf{p}}^{(\text{el})} \equiv (\mathbf{q} \cdot \mathbf{k})c_k + (\mathbf{q} \cdot \mathbf{p})c_p$ , with  $\mathbf{p} \equiv \mathbf{q} - \mathbf{k}$  and the direct correlation function  $c_k$ , is the conventional vertex function, and  $V_{q,\mathbf{k},\mathbf{p}}^{(\text{vis})}$  is the dissipative vertex function, whose explicit form is given by

$$V_{q,\mathbf{k},\mathbf{p}}^{(\text{vis})\lambda} \equiv \frac{n}{m} \int d^3\mathbf{r} g(r) \mathcal{F}(r) \frac{\mathbf{q} \cdot \mathbf{r}}{r^2} r^\lambda (e^{i\mathbf{p} \cdot \mathbf{r}} - e^{i\mathbf{k} \cdot \mathbf{r}}). \quad (19)$$

Note that Eq. (19) includes  $g(r)\mathcal{F}(r)$  in the integrand, similarly to Eqs. (13) and (14). An important property of the dissipative memory kernels is that  $\bar{M}_q^{(2)}(\tau)$  and  $\bar{M}_q^{(3)}(\tau)$  are of opposite sign with respect to  $\bar{M}_q^{(1)}(\tau)$ . This implies that the interparticle dissipation operates to destroy the plateau of the density time-correlator in the  $\beta$ -relaxation regime. These features are commonly seen in the three terms of  $\bar{M}_q^{\lambda\lambda}(t)$  as well.

## NUMERICAL CALCULATION

Now we present the result of the numerical calculation. We first describe the calculational conditions, starting with the non-dimensionalization scheme. The units of mass, length, and time are chosen to be  $m$ ,  $d$ , and  $\tau_0 \equiv d/v_0$ , respectively, where  $v_0 \equiv v_0^{(+)} - v_0^{(-)} = L\dot{\gamma}$  is the relative velocity between the shear boundaries. In these units, the shear rate  $\dot{\gamma} = v_0/L$  is non-dimensionalized as  $\dot{\gamma}^* \equiv \dot{\gamma}\tau_0 = d/L$ , which we require to be small enough, i.e.  $d/L \ll 1$  [27]. In the remainder, non-dimensionalized quantities are denoted with superscript  $*$ .

Next, it is necessary to establish the relation between the bare viscous coefficient  $\zeta$  and the repulsive coefficient  $e$  to compare our result with molecular dynamics simulations. As explained in Ref. [28],  $e$  is related to  $\zeta^*$  as  $e = \exp[-\zeta^* \tau_c^*]$ , where  $\tau_c^* \equiv \pi/\sqrt{2k^* - \zeta^{*2}}$  is the contact duration time of spheres, if the contact force can be approximated by the linear spring model. Here,  $k^*$  is the elastic spring coefficient of  $\mathbf{F}^{(\text{el})}$ . In granular liquids, the steady-state temperature is determined by the balance of the work by shearing and the interparticle dissipation. The case of interest might be where the steady-state temperature is of the same order of the initial equilibrium temperature. In this case,  $\dot{\gamma}^*$  and  $\zeta^*$  are not independent, and must satisfy a certain scaling relation. This relation is obtained by requiring  $\dot{\gamma}^{*2} \simeq 1 - e^2$ , which leads to

$$\zeta^* \simeq \frac{\dot{\gamma}^{*2}}{2\tau_c^*}. \quad (20)$$

We adopt this scaling relation, with  $\tau_c^* = 10^{-4}$ , which is determined by the choice of  $k^*$ .

In Fig. 1, the results for the density time-correlator  $\Phi_q(t)$  and the density-current time-correlator  $\Psi_q(t)$  are shown. The shear rate is  $\dot{\gamma}\tau_0 = 10^{-2}$ , the volume fraction  $\phi$  is  $\varepsilon \equiv (\phi - \phi_c)/\phi_c = +10^{-3}$ , where  $\phi_c \simeq 0.516$  is the

critical MCT transition point in equilibrium, and  $\zeta$  is varied, which corresponds to varying  $e$ . It can be seen that  $\Phi_q(t)$  is almost coincident for  $\zeta^* \leq 1.0$ , which implies that the effect of dissipation is negligible. However, for  $\zeta^* > 1.0$ , which corresponds to the case of  $e < 0.9999$ , the plateau of  $\Phi_q(t)$  is destroyed, and  $\Phi_q(t)$  converges to the Debye-type relaxation curve at  $\zeta^* \simeq 2.0$ , i.e.  $e \simeq 0.9998$ . This drastic demolishing of the plateau is mainly caused by the dissipative memory kernels  $\bar{M}_q^{(2)}(\tau)$  and  $\bar{M}_q^{(3)}(\tau)$ , Eqs. (17) and (18), which are of the opposite sign compared to  $\bar{M}_q^{(1)}(\tau)$ , as mentioned previously. Intuitively, this feature can be regarded as the exhaustion of the “cage” due to inelastic collisions, which enables the particles to escape. Note that the demolishing of the plateau is accomplished at  $t \sim 10\tau_0$ , which is far below the  $\alpha$ -relaxation time  $\tau_\alpha \sim 10^2\tau_0$ , where the effect of shear becomes significant. This may justify the application of the isotropic approximation.

Furthermore, it is remarkable that, complementarily to  $\Phi_q(t)$ , a plateau emerges in the tail of  $\Psi_q(t)$  for  $\zeta^* > 1.0$ . This implies that the density-current correlation is essential to the demolishing of the plateau of  $\Phi_q(t)$ , which supports the role of the dissipative memory kernels,  $\bar{M}_q^{(2)}(\tau)$  and  $\bar{M}_q^{(3)}(\tau)$ .

The obtained result is compatible with the result from molecular dynamics, which also indicates that the plateau of the density time-correlator disappears for  $e < 0.99$ , while it recovers for the nearly elastic case [29].

## CONCLUDING REMARKS

It is notable that the projection onto the density-current modes, Eq. (5), plays an essential role. This is in contrast to the sheared thermostatted systems, where the effect of  $\mathcal{P}_{nj}(t)$  has been proved to be negligible [26]. This difference resides in the nature of the dissipative interaction, i.e. whether it is single-body or two-body.

According to the integration-through-transient scheme of Ref. [30], it is able to derive a formula for the steady-state shear stress in terms of time-correlators. Then, we can obtain the constitutive equation for the shear stress, which is to be compared to the result of molecular dynamics [6, 7]. This issue, with an analysis near the jamming transition point, will be published elsewhere [25].

In conclusion, we have successfully formulated a MCT for sheared granular liquids. We have demonstrated that the plateau of the density time-correlator disappears for  $e < 0.9999$ , as observed in molecular dynamics simulations. This destruction of the plateau results from the effect of the density-current correlation.

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